

Cumulant t -expansion for strongly correlated fermions

A. K. Zhuravlev*

Institute of Metal Physics, 620990 Ekaterinburg, Russia

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A systematic nonperturbative scheme is implemented to calculate the ground state energy for a wide class of strongly correlated fermion models. The scheme includes: (a) method of automatic calculations of the cumulants of the model Hamiltonian; (b) method of the ground state energy calculation from these cumulants using the t -expansion proposed by Horn and Weinstein [Phys. Rev. D **30**, 1256 (1984)] with new procedure of its extrapolation to $t \rightarrow \infty$. As an example of application of the method all cumulants up to the 8-th order for spinless fermion model are calculated exactly, and converging sequences of approximations to the ground state energy are obtained for one-, two- and three-dimensional versions of the model.

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I. INTRODUCTION

The problem of strongly correlated quantum many-body systems is one of the most complicated in theoretical physics. With the exception of a few of simplified models this problem cannot be solved analytically, so that one must resort to numerical methods. But here a researcher is faced with serious difficulties. For example, exact diagonalization runs into the exponential growth of the Hilbert space dimension with increasing size of the system and therefore is limited to small clusters, even when using the Lanczos algorithm¹. A more sophisticated Density-Matrix Renormalization Group technique with high-energy states truncation² gives excellent results for the ground state energy of one-dimensional Fermi systems, but has its own limitation when applied to two- and three-dimensional cases³. Quantum Monte Carlo method⁴ can potentially handle larger systems. However, the method works poorly at low temperatures for fermion systems because of the so called “minus-sign” problem⁵.

As an alternative, a certain interest in the construction of regular expansions still exists⁶. The attractive feature of such alternative is the relative simplicity of calculation of terms in the expansion. Unfortunately, the series expansions in powers of the coupling constants usually diverge⁷. However, there are regular expansion methods which are not reduced to power expansion in coupling constant. For example, high-temperature expansion is that one worth to mention⁸.

Another one is the so called t -expansion⁹, which we describe briefly in what follows. Given a Hamiltonian \hat{H} and an initial state $|\phi_0\rangle$, let us define the moments

$$\mu_m = \langle \phi_0 | \hat{H}^m | \phi_0 \rangle \quad (1)$$

($|\phi_0\rangle$ is normalized to unity) and introduce auxiliary function

$$E(t) = \frac{\langle \phi_0 | \hat{H} e^{-\hat{H}t} | \phi_0 \rangle}{\langle \phi_0 | e^{-\hat{H}t} | \phi_0 \rangle} \quad (2)$$

which can be written as a power series in the parameter t :

$$E(t) = \sum_{m=0}^{\infty} \frac{I_{m+1}}{m!} (-t)^m, \quad (3)$$

where

$$I_{m+1} = \mu_{m+1} - \sum_{p=0}^{m-1} \binom{m}{p} I_{p+1} \mu_{m-p} \quad (4)$$

are the cumulants¹⁰ (note that in^{6,11,12} the values I_m were named “connected moments”). Then

$$E_0 = \lim_{t \rightarrow \infty} E(t) \quad (5)$$

is the minimal eigenvalue of the Schrödinger equation

$$\hat{H}|\psi_0\rangle = E_0|\psi_0\rangle \quad (6)$$

provided that $\langle \psi_0 | \phi_0 \rangle \neq 0$ (see⁹ for proof).

There were attempts to use t -expansion in lattice gauge theory¹³, quantum chromodynamics¹⁴, quantum chemistry¹¹. In condensed matter physics t -expansion was applied to the square lattice Heisenberg antiferromagnet^{15,16}. For the models of interacting electrons on a lattice this method is not used mainly for two reasons: 1) it is difficult to calculate cumulants I_n for any realistic model, 2) it is not easy to calculate the limit (5) having the finite number of known cumulants. In this paper we present a solution to both of these problems and test it for the spinless fermion model which is a typical example of strongly correlated fermion models.

II. CALCULATION OF THE CUMULANTS

The Hamiltonian of this model reads

$$\begin{aligned} \hat{H} &= \hat{W} + \hat{V}, \\ \hat{W} &= -w \sum_{i>j} c_i^\dagger c_j + c_j^\dagger c_i, \quad \hat{V} = v \sum_{i>j} c_i^\dagger c_i c_j^\dagger c_j \end{aligned} \quad (7)$$

with i and j being nearest neighbor lattice sites.

The one-dimensional spinless fermion model is equivalent to the exactly solvable spin- $\frac{1}{2}$ XXZ model¹⁷. Therefore the model (7) in one dimension is often used to test new methods of calculations (see, e.g.,²). Note that for the half-filled case of the model the metal-insulator transition takes place with the appearance of the gap in the energy spectrum at $v > 2w$.

If the initial wavefunction $|\phi_0\rangle$ has the form

$$|\phi_0\rangle = \prod_l c_l^\dagger |0\rangle \quad (8)$$

($|0\rangle$ is the state without fermions, l runs over some set of the lattice sites) then many-operator average included in cumulant I_n can be calculated using Wick's pairing technique. We have to

- 1) connect each creation operator c_i^\dagger with one of the annihilation operators c_j with lines by all the ways possible,
- 2) for each way of the connection assign a term with factor $(-1)^P$, where P is the number of connecting lines intersections,
- 3) replace each connected pair of operators c_i^\dagger and c_j (or c_i and c_j^\dagger) by the average $\langle c_i^\dagger c_j \rangle_0$ (or $\langle c_i c_j^\dagger \rangle_0$), where we introduced the notation $\langle \dots \rangle_0 \equiv \langle \phi_0 | \dots | \phi_0 \rangle$.

For example, the calculation of 4-operator average is

$$\begin{aligned} \langle c_i^\dagger c_j c_k^\dagger c_l \rangle_0 &= \langle c_i^\dagger c_j \rangle_0 \langle c_k^\dagger c_l \rangle_0 + \langle c_i^\dagger c_l \rangle_0 \langle c_j c_k^\dagger \rangle_0 \\ &= n_i \delta_{ij} n_k \delta_{kl} + n_i \delta_{il} (1 - n_k) \delta_{jk} \end{aligned} \quad (9)$$

where $n_i = 1$ if i -th site in $|\phi_0\rangle$ is filled, and $n_i = 0$ if the site is an empty one. Thus each average can be computed easily, but there are too many of them to perform all the calculations manually. To complete the task the symbolic manipulation computer program was written that performs these calculations.

To be certain let us consider the one-dimensional half-filled case with the initial state $|\phi_0\rangle = |10101010\dots 10\rangle$. For this state $\hat{V}|\phi_0\rangle = 0$, so that the terms included in $\langle \hat{H}^n \rangle_0$ which begin with or end with the operator \hat{V} vanish altogether. Therefore one obtains simpler expressions for the moments μ_n :

$$\begin{aligned} \mu_1 &= \langle \hat{H} \rangle_0 = \langle \hat{W} \rangle_0, \\ \mu_2 &= \langle \hat{H}^2 \rangle_0 = \langle \hat{W} \hat{W} \rangle_0, \\ \mu_3 &= \langle \hat{H}^3 \rangle_0 = \langle \hat{W} \hat{W} \hat{W} \rangle_0 + \langle \hat{W} \hat{V} \hat{W} \rangle_0, \dots \end{aligned} \quad (10)$$

Substituting (10) into (4) we obtain compact expressions for the cumulants

$$\begin{aligned} I_1 &= \langle \hat{W} \rangle, \\ I_2 &= \langle \hat{W} \hat{W} \rangle_c, \\ I_3 &= \langle \hat{W} \hat{W} \hat{W} \rangle_c + \langle \hat{W} \hat{V} \hat{W} \rangle_c, \dots \end{aligned} \quad (11)$$

where the index “c” means that only connected terms give contribution in pairings like (9), i.e. those in which isolated group of operators \hat{W} and \hat{V} are absent.

Substituting the expressions (7) for \hat{W} and \hat{V} into (11), using Wick's pairing technique and performing necessary analytical calculations with the help of the above-mentioned computer program, we obtain the final expressions for cumulants of the half-filled one-dimensional spinless fermion model:

$$\begin{aligned} I_1 &= 0, \quad I_2 = w^2 N, \quad I_3 = w^2 v N, \\ I_4 &= (-6w^4 + w^2 v^2) N, \\ I_5 &= (-28w^4 v + w^2 v^3) N, \\ I_6 &= (160w^6 - 86w^4 v^2 + w^2 v^4) N, \\ I_7 &= (1704w^6 v - 220w^4 v^3 + w^2 v^5) N, \\ I_8 &= (-9520w^8 + 10736w^6 v^2 - 510w^4 v^4 + w^2 v^6) N \end{aligned} \quad (12)$$

where N is the number of lattice sites. The number of cumulants which could be computed is limited by a computer power only.

III. CALCULATION OF THE LIMIT $E(t \rightarrow \infty)$

The next step is the calculation of the limit (5). In order to calculate this limit one must know all the cumulants, which is impossible for any real system. All that we know about the function $E(t)$ is its finite power series

$$E(t) = \sum_{m=0}^{M+1} \frac{I_{m+1}}{m!} (-t)^m \quad (13)$$

and the following information: 1) the function $E(t)$ is a monotonically decreasing one since the derivative of (2) is the negative of the expectation value of the positive operator $(\hat{H} - \langle \hat{H} \rangle)^2$, i.e. $\frac{dE}{dt} < 0$; 2) $E(t)$ rapidly goes to a constant, hence $\frac{dE}{dt}$ goes to zero as t goes to infinity. The

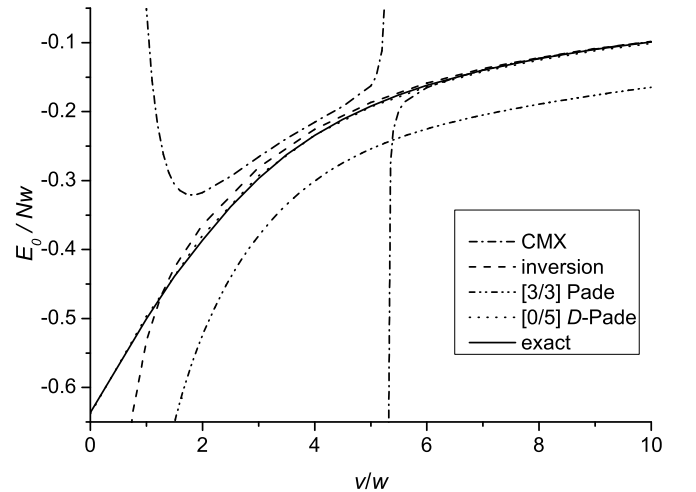


FIG. 1: The ground state energy density for one-dimensional half-filled spinless fermion model calculated by different methods using the cumulants up to I_7

articles^{9,11,12} proposed some ways to calculate the limit

(5) using the above information. The Figure 1 shows the results of several methods of calculating the limit (5) when the first seven cumulants are known: connected-moments expansion (CMX) by Cioslowski¹¹, inversion method by Stubbs¹², diagonal [3/3] Padé approximant for $E(t)$ and [0/5] D -Padé approximations used in the pioneering work⁹. The D -Padé method yields much more accurate results than others and gives a satisfactory results for the model under consideration in the wide range of parameters.

It turns out that there is a method which converges more rapidly compared with D -Padé method. Now we describe it. The ground-state energy required, E_0 , can be obtained from

$$\int_0^\infty E'(t)dt = E(\infty) - E(0) = E_0 - I_1, \quad (14)$$

where $E'(t) \equiv \frac{dE(t)}{dt}$, and we have to find the best way to interpolate the function $E'(t)$ between its known values $E'(0) = -I_2$ and $E'(\infty) = 0$.

Let us expand the initial state $|\phi_0\rangle$ in terms of the eigenfunctions of the Hamiltonian as

$$|\phi_0\rangle = \sum_{n=0}^{\infty} \sqrt{b_n} |\psi_n\rangle \quad (15)$$

with $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$. Then the function $E(t)$ can be rewritten as

$$E(t) = \frac{\int_{E_0}^{E_{\max}} E e^{-Et} \rho(E) dE}{\int_{E_0}^{E_{\max}} e^{-Et} \rho(E) dE}, \quad (16)$$

where $\rho(E) = \sum_n b_n \delta(E - E_n)$. Direct differentiation of (16) shows that the asymptotic behavior of the function $E'(t)$ at $t \rightarrow \infty$ depends on the features of the eigenvalue spectrum. Let us consider the two limiting cases:

- 1) for continuous spectrum with $\rho(E) = \text{const}$ $E'(t) \sim -1/t^2$;
- 2) for discrete spectrum $E'(t) \sim -e^{-\Delta t}$, where Δ is the gap between the ground state energy E_0 and the first excited state energy E_1 .

Now let us consider the function $Q(t) \equiv -I_2/E'(t)$. Its asymptotic behavior must be between $\sim t^2$ and $\sim e^{\Delta t}$. Given the cumulants from I_1 to I_{M+2} , calculating [0/ M] Padé approximant for $E'(t)$ we obtain the series expansion for function $Q(t)$ up to order M :

$$Q_M(t) = 1 + q_1 t + q_2 t^2 + \dots + q_M t^M. \quad (17)$$

If the values q_m are close to the coefficients of expansion of the exponential, i.e. there is a good fit to the dependence

$$q_m \approx \frac{\alpha^m}{m!} \quad (\alpha > 0) \quad (18)$$

(see Fig.2) there is a reason to assume that $Q(t) \sim e^{\alpha t}$ and take into account the contribution by Kummer's se-

ries transformation method¹⁸. Namely, let us introduce

$$\alpha = \frac{1}{M} \sum_{m=1}^M (m! q_m)^{1/m} \quad (19)$$

and replace $Q_M(t)$ by $\tilde{Q}_M(t)$:

$$\tilde{Q}_M(t) = Q_M(t) + e^{\alpha t} - \sum_{m=0}^M \frac{\alpha^m}{m!} t^m \quad (20)$$

where the first M terms of the series for $\tilde{Q}_M(t)$ coincide with $Q_M(t)$. Then an expression for the approximate ground state energy is

$$E_0(I_{M+2}) = I_1 - \int_0^\infty \frac{I_2}{\tilde{Q}_M(t)} dt, \quad (21)$$

The appearance of negative q_m in (17) should be considered as an indication that the function $Q(t)$ has no an exponential asymptotics. Therefore, it has the power asymptotics. Here it is reasonable to use the Padé approximants for $Q(t)$ (or $E'(t)$). For the integral in (14) is finite we can use for $E'(t)$ only approximants like [0/ M], ..., [L/ $M-L$], ... where $M-L \geq L+2$. Since $E'(t)$ is always negative we have to control that this property holds for the Padé approximants. If some approximant has alternating-sign at certain values of L then we will exclude it from consideration. For each of the remaining proper approximants we calculate the ground state energy E_0 according to (14). And if the number of proper approximants is more than one, then we carry out averaging over the energies calculated.

The new extrapolation method described above we call adapted derivative (AD) method.

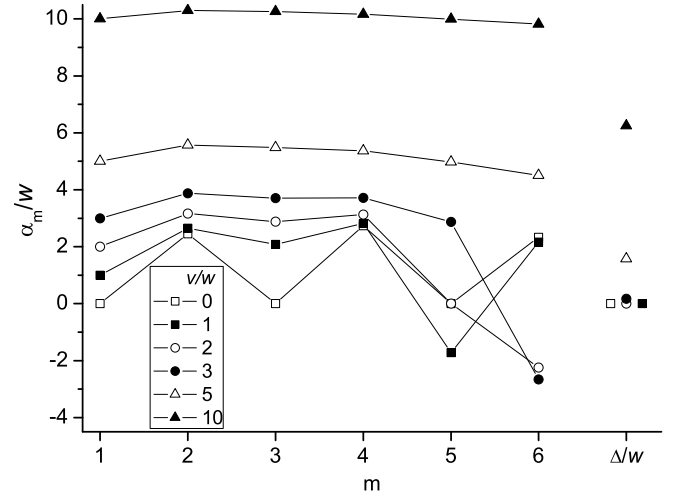


FIG. 2: The quantity $\alpha_m \equiv \text{sgn}(q_m)(m!|q_m|)^{1/m}$ for one-dimensional half-filled spinless fermion model. The right column shows the exact value of the gap Δ in the thermodynamical limit¹⁷

The results of the ground state energy calculations using the described technique are presented in the Tab.I.

As one can see the estimation for the ground state energy converges to its exact value with increasing of the number of the cumulants known. The new AD-method radically accelerates the convergence rate compared to D -Padé approximation for large v/w , that is, where there is a large gap Δ in the energy spectrum, despite the fact that α (19) is only a rough estimate for Δ (see Fig.2). For $v \lesssim w$ the accuracy of the AD-method is comparable to the accuracy of the D -Padé method. The last case is the most difficult for the method provided the particle-hole alternating ordered initial state $|\phi_0\rangle$ is chosen.

TABLE I: The sequences of $[0/M]D$ -Padé and AD approximations to the ground state energy density $E_0/(Nw)$ for one-dimensional half-filled spinless fermion model using the cumulants up to I_{M+2}

v/w	0	2	5	10	20
DP(I_4)	-0.906900	-0.553574	-0.290259	-0.153778	-0.078116
DP(I_5)	-0.906900	-0.422301	-0.215831	-0.113986	-0.057867
DP(I_6)	-0.638353	-0.379567	-0.198060	-0.104281	-0.052850
DP(I_7)	-0.638353	-0.379567	-0.193261	-0.101028	-0.051103
DP(I_8)	-0.625157	-0.382435	-0.191984	-0.099799	-0.050408
AD(I_4)	-0.554850	-0.348868	-0.184327	-0.097832	-0.049721
AD(I_5)	-0.615481	-0.365772	-0.185731	-0.098003	-0.049742
AD(I_6)	-0.635617	-0.363360	-0.187039	-0.098267	-0.049780
AD(I_7)	-0.638353	-0.379567	-0.188228	-0.098438	-0.049802
AD(I_8)	-0.625157	-0.383881	-0.189472	-0.098609	-0.049824
exact	-0.636620	-0.386294	-0.192014	-0.099000	-0.049875

IV. SQUARE AND SIMPLE CUBIC LATTICES

Now let us discuss two- and three-dimensional spinless fermion models, where the exact solutions are not known, except for a case of non-interacting particles $v = 0$. For half-filled spinless fermion model on a square lattice with chessboard ordered initial state $|\phi_0\rangle$ the cumulants are:

$$\begin{aligned}
I_1 &= 0, \quad I_2 = 2w^2N, \quad I_3 = 6w^2vN, \\
I_4 &= (-36w^4 + 18w^2v^2)N, \\
I_5 &= (-488w^4v + 54w^2v^3)N, \\
I_6 &= (3200w^6 - 4516w^4v^2 + 162w^2v^4)N, \\
I_7 &= (96304w^6v - 35576w^4v^3 + 486w^2v^5)N, \\
I_8 &= (-666400w^8 + 1794464w^6v^2 - 257044w^4v^4 \\
&\quad + 1458w^2v^6)N.
\end{aligned} \tag{22}$$

The results for the ground state energy density is presented in Fig.3 and Tabl.II.

For half-filled spinless fermion model on the simple cubic lattice with “three-dimensional chessboard” ordered initial state $|\phi_0\rangle$ the cumulants are:

$$\begin{aligned}
I_1 &= 0, \quad I_2 = 3w^2N, \quad I_3 = 15w^2vN, \\
I_4 &= (-90w^4 + 75w^2v^2)N,
\end{aligned}$$

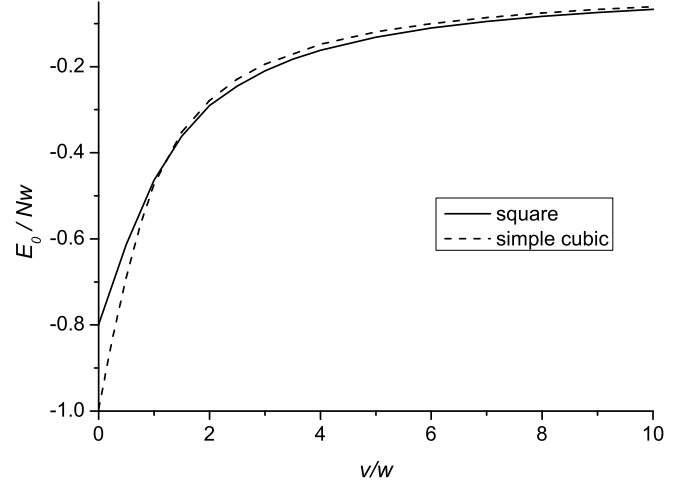


FIG. 3: The ground state energy density for half-filled spinless fermion model on square and simple cubic lattices

TABLE II: The sequences of $[0/M]D$ -Padé and AD approximations to the ground state energy density $E_0/(Nw)$ for half-filled spinless fermion model on square lattice using the cumulants up to I_{M+2}

v/w	0	2	5	10	20
DP(I_4)	-1.047198	-0.450341	-0.203638	-0.103968	-0.052265
DP(I_5)	-1.047198	-0.334617	-0.150765	-0.076991	-0.038708
DP(I_6)	-0.771728	-0.304991	-0.137671	-0.070281	-0.035330
DP(I_7)	-0.771728	-0.296680	-0.133138	-0.067926	-0.034141
DP(I_8)	-0.794703	-0.293364	-0.131316	-0.066976	-0.033662
AD(I_4)	-0.874327	-0.299360	-0.130763	-0.066336	-0.033292
AD(I_5)	-0.971901	-0.292527	-0.130079	-0.066244	-0.033280
AD(I_6)	-0.767748	-0.289574	-0.129868	-0.066218	-0.033277
AD(I_7)	-0.771728	-0.289911	-0.129840	-0.066212	-0.03327588
AD(I_8)	-0.799582	-0.290245	-0.129841	-0.066211	-0.03327581
exact	-0.810569				

$$\begin{aligned}
I_5 &= (-2052w^4v + 375w^2v^3)N, \\
I_6 &= (14880w^6 - 32058w^4v^2 + 1875w^2v^4)N, \\
I_7 &= (744600w^6v - 427572w^4v^3 + 9375w^2v^5)N, \\
I_8 &= (-6083280w^8 + 23234064w^6v^2 \\
&\quad - 5240898w^4v^4 + 46875w^2v^6)N.
\end{aligned} \tag{23}$$

The results for the ground state energy density is presented in Fig.3 and Tabl.III.

In both cases, the approximations sequence converge, behaving similarly to the one-dimensional case.

V. CONCLUSIONS

As we have seen, the present method yields converging sequence of approximations to the ground state energy of a typical strong-correlated many-fermion model. Seemingly, the sequence of approximations will converge for

TABLE III: The sequences of $[0/M]D$ -Padé and AD approximations to the ground state energy density $E_0/(Nw)$ for half-filled spinless fermion model on simple cubic lattice using the cumulants up to I_{M+2}

v/w	0	2	5	10	20
DP(I_4)	-1.216734	-0.427777	-0.185303	-0.093840	-0.047073
DP(I_5)	-1.216734	-0.317453	-0.137238	-0.069500	-0.034864
DP(I_6)	-0.970781	-0.290241	-0.125303	-0.063438	-0.031820
DP(I_7)	-0.970781	-0.281633	-0.121129	-0.061306	-0.030749
DP(I_8)	-0.991937	-0.278155	-0.119448	-0.060446	-0.030317
AD(I_4)	-1.015876	-0.280232	-0.118592	-0.059821	-0.029978
AD(I_5)	-1.129247	-0.275983	-0.118229	-0.059773	-0.029972
AD(I_6)	-0.963441	-0.274673	-0.118121	-0.059759	-0.029970
AD(I_7)	-0.970781	-0.274901	-0.118099	-0.059756	-0.0299692
AD(I_8)	-0.995160	-0.275095	-0.118096	-0.059755	-0.0299691
exact	-1.002420				

any Hamiltonian whose moments (1) are finite. The generalization of the method to the case of real electrons with spin is very simple: one needs to pair only the operators with the same spin indices in the formulas like (9). Therefore the method is applicable to real many-electron problems in condensed matter physics and quantum chemistry. The method is of interest for researchers because it gives a systematic approach to physical problems with strong interaction, which does not require the smallness of the interaction. The AD-method which we introduce to calculate the limit $E(t \rightarrow \infty)$ can be useful in the traditional areas of the t -expansion application, like the lattice gauge theory and quantum chromodynamics.

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* Electronic address: zhuravlev@imp.uran.ru

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